Optimization of distillation column reflux ratio for distillate purity and process energy requirements

Article *in* International Journal of Basic and Applied Science · September 2023

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International Journal of Basic and Applied Science 12 (2) (2023) 72-81

Published by: IOCSCIENCE

International Journal of Basic and Applied Science

Journal homepage: www.ijobas.pelnus.ac.id

Optimization of distillation column reflux ratio for distillate purity and process energy requirements

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Article Info

Article history:

Received Aug 9, 2023
Revised Aug 20, 2023
Accepted Sep 28, 2023

Keywords:

Aspen hysis;
Bubble point;
Carboxymethyl cellulose;
Ethanol purification;
Reboiler steam.

ABSTRACT

Recovering ethanol solutions from filtration, extraction, and stripping operations is done in the distillation column, a separation process unit in the carboxymethyl cellulose production plant. Because the ethanol produced by these techniques is produced at a lower concentration, distillation is required to purify the ethanol. This procedure can raise the concentration of ethanol by separating it from the mixture. The concentration of the ethanol solution needs to be 85% in order to be reused. This case study aims to determine the optimal reflux ratio for a distillation column, model the process in both real-world and manual calculation scenarios using Aspen Hysys software, and evaluate the effects of increasing the reflux ratio. Manual computations yielded a reflux ratio result of 0.91814. In the meantime, an ethanol concentration of 85% is produced by the reflux ratio of 1.080 that is derived from the Aspen Hysys simulation. By generating a heat flow of 1.889 x 10^6 kJ/h, the ideal reflux ratio of 1.080 was reached, whereas the Aspen Hysys simulation yielded a reflux ratio of 0.91814. This allowed for an ethanol concentration of 85%. The Aspen Hysys simulation yields an ethanol concentration of 82.11% and a heat flow of 1.399 x 10^6 kJ/h. The ethanol concentration and reboiler steam heat flow are impacted by the reflux ratio value, according to the reflux ratio results. The amount of reboiler steam heat generated may become linear with a larger reflux ratio, and the energy required to complete the distillation process may likewise rise.

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1. INTRODUCTION

Distillation is the method of dividing a mixture of substances based on stark variations in boiling point and vapor pressure [1]. The distillation column is one of the complex pieces of process equipment for modeling and controlling important parts of a separation and purification process that is often used by the chemical industry [2], and one of them is in the Carboxymethyl Cellulose (CMC) manufacturing plant (thickening agent) in the Bekasi district area. This unit helps continue the ethanol solution recovery process. Based on internal data from the CMC industry in Bekasi district, this CMC chemical is a solution resulting from the filtration, extraction, and stripping process that is stored in a storage tank with a lower ethanol concentration. The same information states that reuse of ethanol solution either as a reaction medium in the reactor or for the washing process during the production of purified type CMC, if this chemical has a concentration of 85%. To achieve this concentration, the distillation column unit is a separation process between ethanol and the mixture. The upper output from the distillation column is ethanol, with smaller quantities of other components. This distillate undergoes a condensation process through condenser equipment, and the output goes to a temporary storage tank. Part of the distillate is refluxed to increase the concentration of the ethanol solution.

During the distillation process, temperature, distillation column pressure, and reflux ratio are factors that influence the quantity and concentration of the distillate produced. The distillation column's condensate return rate to the amount of recovered distillate is known as the reflux ratio. The presence of reflux will have the effect of increasing the concentration of the distillate. The purity of the components resulting from the separation process through a distillation column becomes effective and efficient by paying attention to the reflux ratio [3]. If the reflux ratio is too low, it can result in an improper component separation process (far from the process output target) and produce an impure fraction (still containing other unwanted components). On the other hand, a reflux ratio value that is too high can slow down the process of separating the mixture components and become inefficient, but the output has high purity [4]. Apart from that, increasing the reflux ratio also has an impact on the amount of energy consumed in the distillation column [5]. Apart from that, the contribution of a combination of pressure factors and reflux ratios is also included in the study of the distillation process unit [6]. Of course, this blending step also aims to obtain the required purity of the distillate product and minimize heat usage for the reboiler because the distillation column is one of the operating units that consumes a lot of energy [7].

The study of the use of reflux ratios in distillation columns involves the use of mathematical equations and process simulations through software to optimize the level of purity of the ethanol solution. Aspen Hysys is an engineering software that helps complete the simulation of a series of chemical industrial processes by modeling a process system in detail [8], [9]. This program is a process modeling tool for air separation units, gas processing, petroleum product and derivative refining, conceptual design, process optimization, and performance reviews [10]. Other applications result in the modeling of several chemical industrial processes, such as those related to oil and gas, oil refineries, heavy industry, petrochemical industry, natural gas processing plants, synthesis gas generation, ethanol factories, biodiesel factories, and so forth [11]. For precise estimates of physical parameters, transport properties, and phase behavior in the oil and gas industry as well as refining processes, Aspen Hysis offers a comprehensive set of fundamental thermodynamic principles [12]. Other complete features include modeling various operating units such as separators, reactors, streams, heat transfer, rotating, piping, logic, optimizers, subflowsheet operations, as well as utilities in steady state and dynamic conditions [13], [14]. The application of this simulation becomes a bridge for implementing research activities with industry practitioners [15] and attracts implementation opportunities for other software implemented by companies in the field of chemical engineering [16].

The main advantage of using Aspen Hysys is that it can save time in carrying out a number of calculations in designing a complicated and complex process compared to using mathematical equations. Aspen Hysis simulation is additionally advantageous from an optimization standpoint, allowing for much lower engineering costs and better operational decisions to improve plant performance and profitability [17]. Therefore, this study aims to determine the effect of distillation column product purity concentration and reboiler steam heat flow on increasing reflux ratios. During the research, the aspen hysys simulation process was utilized as a comparison to the use of mathematical equations to examine the two points of research objectives.

2. RESEARCH METHOD

This research is a dry study that runs the distillation process through the use of Aspen Hysis computational software. This step is aimed at comparing the results of process simulation against the use of mathematical equations (Equation 1-10) below. The focus of this research is on increasing the reflux ratio value (R_m = 1.2 – 1.5) from actual industry data processed into the mathematical equations and also the computational simulation. The results of the distillation column simulation can be used to determine the ethanol concentration obtained and the heat requirement of the reboiler steam using the reflux ratio value from the results of manual calculations and aspen hysys simulation results to get optimal results.

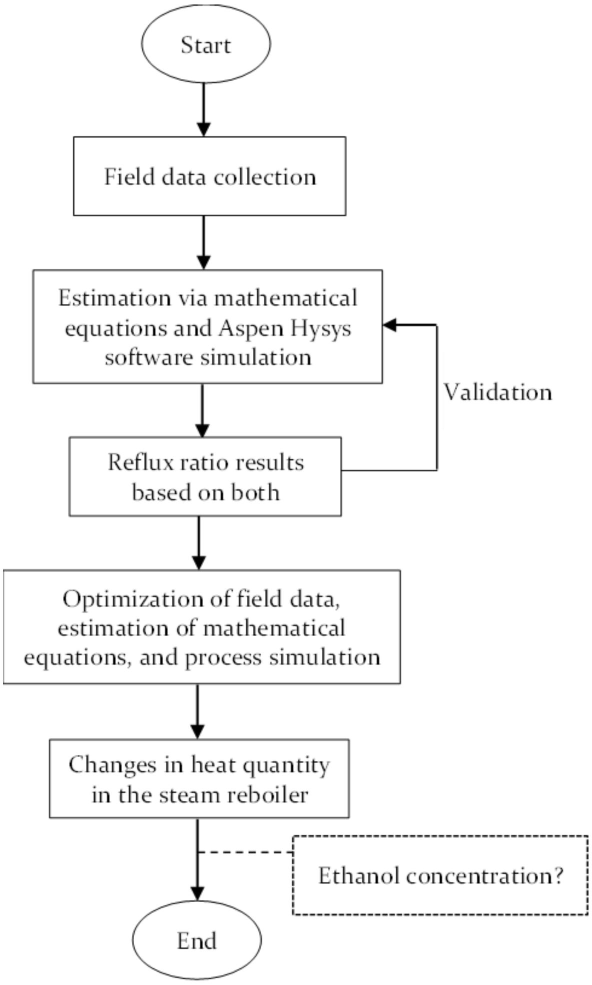

Figure 1. Steps to optimize distillation unit performance in the CMC industry

Data on the operating conditions of distillation columns at thickener companies are the result of direct observations via the Distributed Control System (DCS) monitor and the result. The information includes the components that need to be separated, the operating circumstances, the make-up of the feedstock, the distillate, and the bottom products, as well as the quantity of trays used and the reflux ratio during the distillation process. Mathematical equations (1) to (10) and the Aspen Hysis software are used to calculate the reflux ratio when ethanol is separated from a mixture of other components. The CMC chemical factory does not yet display actual field data regarding the reflux ratio used, so the predicted range is an opportunity to obtain optimum conditions from a given increase in the reflux ratio.

Based on field data for distillation columns, mass balances, both overall and per component, require feed mass flow rate data and properties such as density data through instructions [17], [18].

$$\dot{M} = \rho \times \dot{V} \tag{1}$$

Operating conditions for the upper and lower parts of the distillation column include:

Overall mass balance $$F = D + W \tag{2}$$

Mass balance per component $$F\, x_{F,i} = D\, x_{D,i} + W\, x_{W,i} \tag{3}$$

Bubble temperature and dew point:

Bubble point condition $$\sum y_i = \sum K_i\, x_i = K_C \sum \alpha_i\, x_i = 1 \tag{4}$$

Dew point condition $$\sum x_i = \sum \left(\frac{y_i}{K_i}\right) = \left(\frac{1}{K_C}\right) \sum \left(\frac{y_i}{\alpha_i}\right) = 1 \tag{5}$$

To obtain these two temperatures involves the role of [18] through trial and error. Then, estimation of vapor pressure A, B, and C variable used the Antoine's data from Table 1 below.

$$\log_{10} P^* = A - \frac{B}{(T + C)} \tag{6}$$

$$\alpha_{L,av} = \sqrt{\alpha_{L,D} \times \alpha_{L,W}} \tag{7}$$

Table 1. Actual data on distillation column operating conditions [18]

Parameter	A	B	C
C2H5OH, ethanol	8.12875	1,660.8713	238.131
H2O	8.055735	1,732.6425	233.08
NaOH	7.46511	7,606.4353	280.16

The need for N_m and R_m for distillation columns involves the role of equations (8) to (10) [18].

$$N_m = \frac{\log \left[\left(\frac{x_{L,D}\,.\,D}{x_{H,D}\,.\,D}\right)\left(\frac{x_{H,W}\,.\,W}{x_{L,W}\,.\,W}\right)\right]}{\log(\alpha_{L,av})} \tag{8}$$

$$R_m + 1 = \sum \frac{\alpha_i\,.\,x_{D,i}}{\alpha_i - \theta} \tag{9}$$

$$1 - q = \sum \frac{\alpha_i\,.\,x_{F,i}}{\alpha_i - \theta} \tag{10}$$

The variable used in the Aspen Hysis simulation is the reflux ratio, which comes from factory data. Calculation results through mathematical equations and evaluation through the use of chemical engineering software using distillate yield data (85% ethanol). The working distillation column has a total condenser type shown in Figure 2.

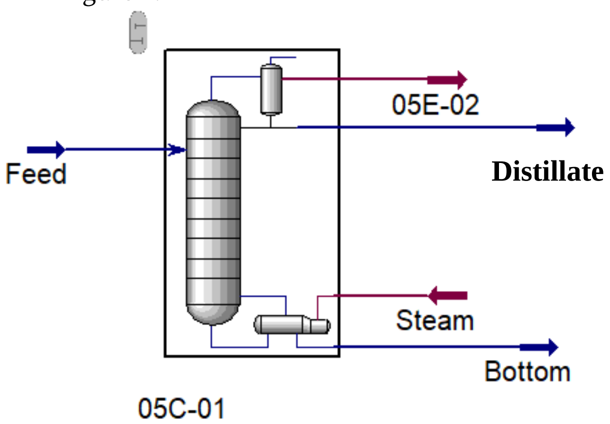

Figure 2. Distillation column purification of ethanol products [19]

Utilizing the Aspen Hysis simulation has a sequence of work steps, namely inputting components, selecting fluid packages, and filling in simulation data for the operating conditions of the feed and distillation columns, which are presented in Table 2. The NRTL (Non-Random Two Liquid) thermodynamic equation is an option for the performance of the purification process for ethanol in the CMC industry. The process system occurs on a large boiling point scale between components. This turns NRTL into a simultaneous solution step for the range of boiling points or concentrations between components, as well as the vapor-liquid equilibrium (VLE or Vapor Liquid Equilibrium) and the liquid-liquid equilibrium (LLE or Liquid-Liquid Equilibrium) [13].

3. RESULTS AND DISCUSSIONS

Based on data from the food additive industry (Table 2), the ethanol solution reused for the production process has a concentration of 85%. To achieve this concentration value, the company uses a reflux ratio value in the range of 2–8. The result of using the mathematical equation (referring to Equations 1–11) gives a reflux ratio value of 0.91814 (see Figure 3). This value is the beginning of the application for the use of Aspen Hysis software. Through the use of the simulation process, an ethanol purity of 82.11% was obtained. The difference in results is found in the use of mathematical equations and process simulations. When inputting data on ethanol purity of 82.11%, the reflux ratio value increased from 0.91814 to 1.080 (see Figure 4). This achievement shows that increasing the reflux ratio value has an effect on the purity concentration of the distillation column product and the reboiler steam heat flow [20]. The application of two ratios through the Aspen Hysis simulation is presented in Figures 3 to 6.

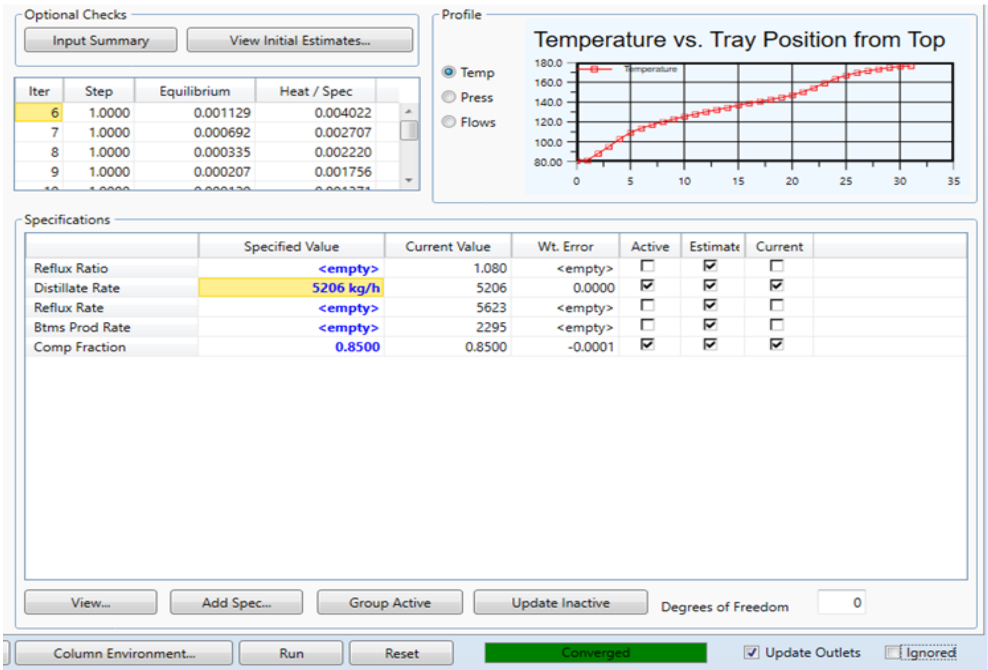

Figure 3. Reflux ratio results (equal to 0,91814) in the Aspen Hysys simulation

To determine the ethanol concentration by using the reflux ratio obtained from the mathematical equation, namely by changing the variable specified value of reflux ratio and activating it. As for the specific value variable, the ethanol concentration is disabled. The result of this step is shown in Figure 4.

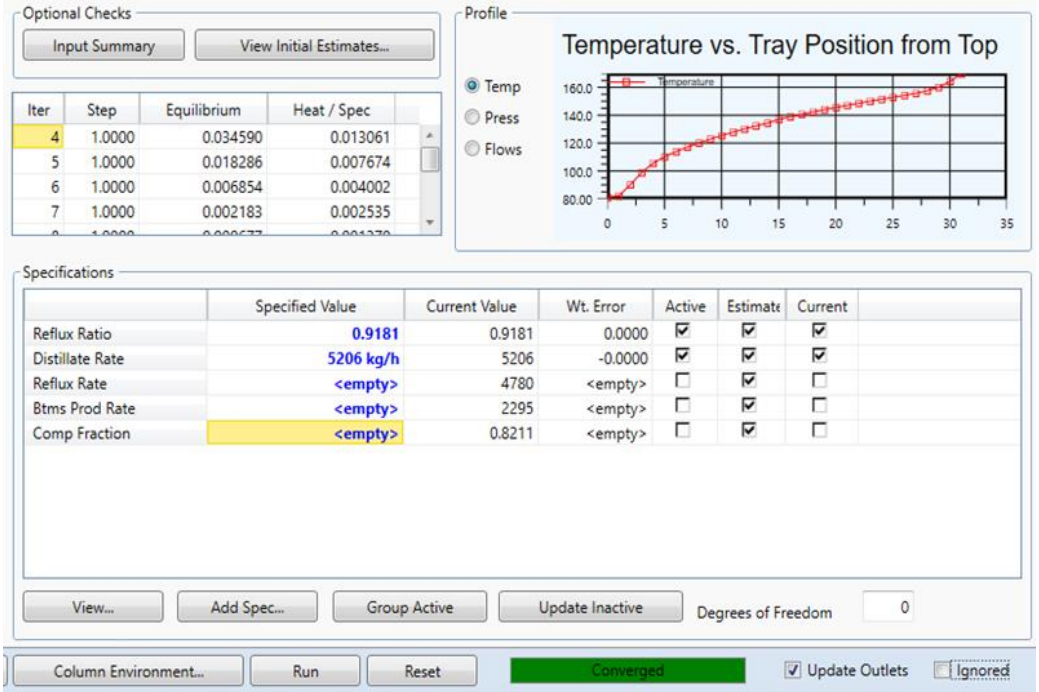

Figure 4. Ethanol concentration results using reflux ratio (equal to 1,080)

Table 2. Actual data on distillation column operating conditions and the results

Parameter	Feed, F	Distillate, D	Bottom, W
Temperature, °C	87	78.70	102
Pressure, bar	0.003	1.1	9
Volumetric flow rate, $\dot{V}$, m^3/h	8.9	6.5864*	2.3136*
Composition, %			
C_2H_5OH, ethanol	59	85	0.01*
H_2O	38.5	15	91.81*
NaOH	1.46		4.77*
$NaCH_3COO$	0.06		0.2*
CMC	0.005		0.002*
Na-glycolate	0.97		3.17*
Na-monochloroacetate	0.005		0.02*

Note: *Data is presented quantitatively from the thickener industry (calculated results)

The concentration of purity of the top and bottom products in the distillation column is one result of increasing the reflux ratio value. Higher reflux ratios are typically employed in the distillation column process to achieve higher product purity [21]–[23] . Meanwhile, if there is no reflux, no contact will occur, and the condensation of the top product obtained will not be large [5]. Figure 5 is the result of data processing through simulation.

Figure 5 shows the optimum reflux ratio results obtained from the simulation of 1.080, with the distillate and bottom concentration results being 85% ethanol and 91.81% water, respectively. The greater the value of the reflux ratio, the concentration of distillate and bottom products will increase. However, the use of a reflux ratio (R = 1.5–8) results in the ethanol concentration in the distillate and the amount of water at the bottom being more likely to be constant. This is caused by the highest degree of separation of a component from the mixture [23], [24]. Increased liquid flow in the distillation column and more opportunities for contact between the vapor and liquid phases can result from an increase in the reflux ratio. However, the greater the value of the reflux ratio, the more likely it is that the component separation process will take place slowly and inefficiently [25].Another effect of increasing the reflux ratio value is on the reboiler steam heat flow. The reboiler is a heat source whose load depends on the amount of liquid being evaporated, and the amount of liquid depends on the size of the reflux ratio [26]. The reflux ratio affects the amount of heat flow from the reboiler. The Aspen Hysis simulation results displayed in Figure 6 below support this.

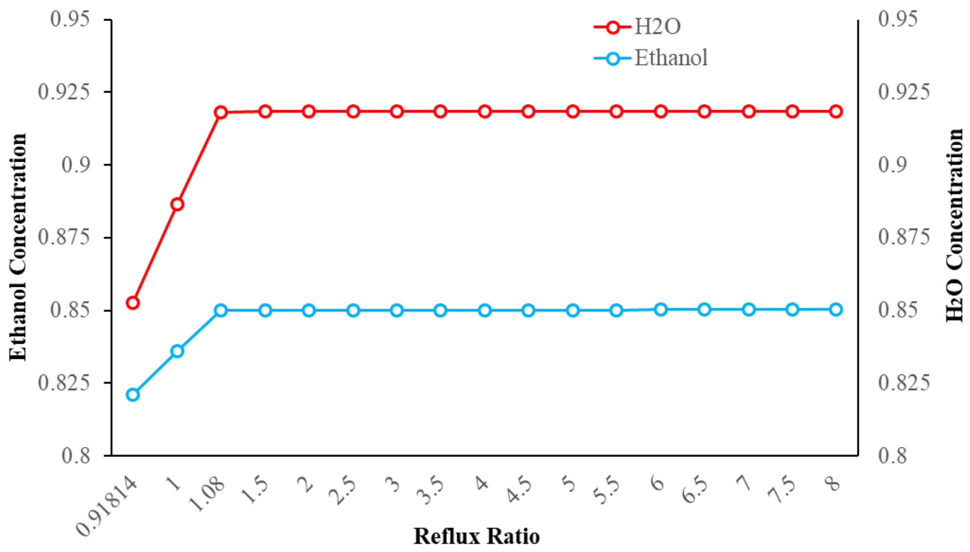

Figure 5. Effect of reflux ratio on distillate and bottom products

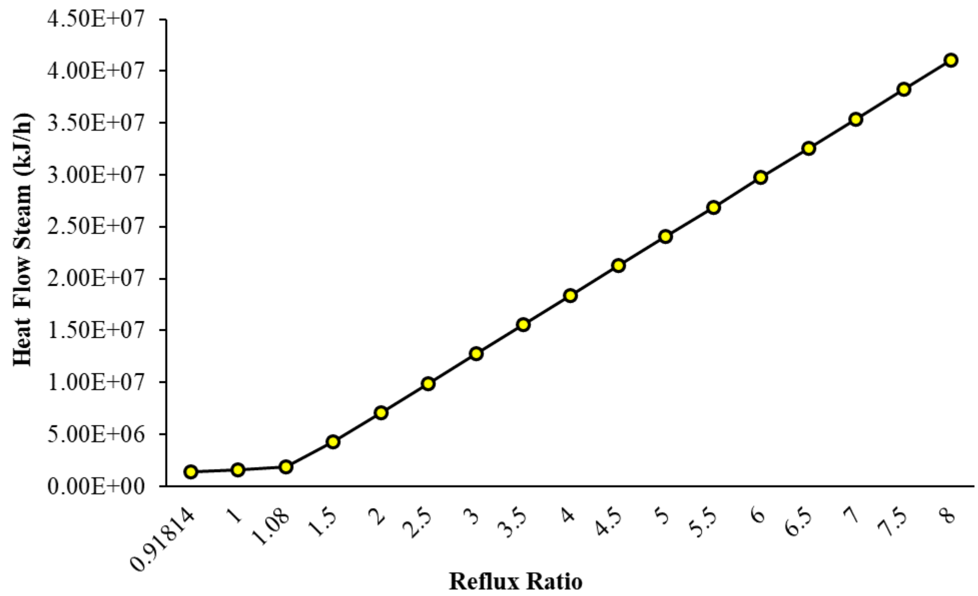

Figure 6. Effect of reflux ratio on heat demand from steam

Figure 6 displays the reflux ratio's results under ideal circumstances, namely 1.080 with a steam reboiler heat requirement of 1.889×10^6 kJ/h. This indicates that the greater the value of the reflux ratio, the more it has a directly proportional impact on the production of reboiler steam heat flow and will, of course, require much greater energy consumption. This heat flow experiences a drastic increase with an increase in the ratio value due to the quantity of liquid returning to the distillation column, so that the heat supply for the reboiler is also greater and also has an impact on the capital of the related industry [27]. Apart from that, if you maintain a higher reflux ratio, you will also need high process operational costs [18]. Then, increasing the energy supply provided by the reboiler can also increase the load on the condenser [28].

4. CONCLUSION

From activities in the thickener industry (CMC), it was found that the optimum reflux ratio ranged from 0.91814 to 1.080 for the ethanol product purity range of 82.11–85%, both through the application of mathematical equations and successive simulations of the Aspen Hysis process. These two values require a steam supply range for the reboiler of $1.399 - 1.889 \times 10^6$ kJ/h. CMC production with an optimum reflux ratio will provide the same for increasing ethanol concentration. Above this ratio will provide similar (constant) product purity and have the opposite effect in the form of slowing down the component separation process (the process is inefficient). The continuation of this research will be a further study to obtain more optimal purification results. Temperature and pressure conditions during the use of the distillation column for ethanol purity are considerations for the utility unit segment and energy supply in carrying out the separation process.

ACKNOWLEDGEMENTS

The writing team would like to thank the CMC company in Bekasi Regency, West Java, for helping and allowing the writing of this article.

NOTATIONS

$\dot{M}$		mass flow rate	kg/h
ρ		density	kg/m³
$\dot{V}$		volumetric rate	m³/h
F	:	flow rates for feed	kg/h
D	:	flow rates for distillate	kg/h
W	:	flow rates for bottom	kg/h
x_F	:	the component compositions for feed	
x_D	:	the component compositions for distillate	
x_W	:	the component compositions for bottom	
x_i	:	the component compositions in liquid phase	
y_i	:	the component compositions in vapor phase	
K_C	:	equilibrium constant	
K_i	:	equilibrium coefficient distribution	
α_i	:	component volatility	
P*	:	vapor pressure	mmHg
T	:	temperature	°C
A, B, and C	:	Antoine constants for several chemical compounds involved	
$\alpha_{L,av}$	:	average volatility	
$\alpha_{L,D}$	:	the component volatilities for light key distillate	
$\alpha_{L,W}$	:	the component volatilities for light key bottom	
N_m	:	minimum number stage	
$x_{L,D}$	:	the component composition for light key distillate	
$x_{H,D}$	:	the component composition for heavy key distillate	
$x_{L,W}$	:	the component composition for light key bottom	
$x_{H,W}$	:	the component composition for heavy key bottom	
R_m	:	minimum reflux ratio using the Underwood method	
q	:	the line intersection between feeds (q − line)	
θ	:	parameter, where this value is obtained through trial and error steps	

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